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The research described in this Final Report includes theoretical studies of the deexcitation of multiply ionized atoms, extensive computations of binding and transition energies including relaxation, relativistic and quantum-electrodynamic effects, and experimental studies of electron correlation through x-ray scattering with synchrotron radiation.

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Atomic Inner-Shell Transitions

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FINAL REPORT

U. S. ARMY RESEARCH OFFICE

GRANT DAHC04-75-G-0021

October 31, 1977

1. Introduction

This is the final report on research performed under U.S. Army Research Office Grant DAHC04-75-G-0061, entitled "Atomic Inner-Shell Transitions." The work was also supported in part by the National Aeronautics and Space Administration under Grant NGR 003-036. In particular, the CDC 7600 computer facility at the Ames Research Center, NASA, was used for many of the numerical computations included in this work.

2. Problems Studied

Aspects of atomic inner-shell physics have been studied with modern techniques. The deexcitation of atoms with multiple inner-shell vacancies has been examined from a fresh point of view. Binding and transition energies have been calculated using high-powered computers that permit the inclusion of relaxation, relativistic, and quantum-electrodynamic effects. The scattering of x rays from molecular hydrogen and from helium has been measured with the intense photon beam from a synchrotron radiation source, and the results have been interpreted in terms of electron correlation. The present state of knowledge of atomic inner-shell processes and of orbital electron capture by the nucleus have been surveyed in comprehensive reviews.

3. Summary of Most Important Results

3.1 Multiplet effects in the decay of multiply ionized atoms

In an atom that contains several inner-shell holes, the vacancies couple to form a multiplet structure. The decay properties of such a system depend critically on the state. Early calculations of fluorescence yields, i.e., of the ratio of radiative to Auger decay rates, disagreed grossly with experiment.

We were able to resolve the discrepancy between calculated and measured fluorescence yields by reexamining the basic underlying definitions. We calculate the Auger and x-ray widths of each multiplet state, compute the individual multiplet fluorescence yields, and find a suitable average. Because the Auger channel is closed for some multiplets in configurations of highly stripped atoms, such states have very large fluorescence yields. This effect was not taken into account in earlier calculations. The present theoretical x-ray yields are much larger, for high charge states, than those calculated previously, and agree extremely well with measurements on ion-atom collision systems. The new theoretical transition probabilities allow a more accurate analysis of experimental results and hence can lead to a better understanding of ion-atom collision mechanisms. For example, comparison with experiment shows that multiplet states are populated statistically in collisions of 35-MeV O^{5+} with Ne, but that sequential stripping occurs when Ne is bombarded with O^{8+} or Cl^{13+} ions. The extreme variation among properties of individual multiplet states is illustrated by the fact that the theoretical L_1 x-ray yield of Ar ions containing 6 M-shell vacancies is more than 400 times larger for an atom that is statistically ionized than for a sequentially stripped atom. Our theoretical studies of the deexcitation of multiply ionized atoms have been extended to include calculations for selected configurations of Li-like Ne and of multiply ionized S and Cl, identifying relatively long-lived states of very high x-ray yields that may become promising candidates in schemes for producing amplified stimulated emission in the x-ray range.

3.2 Feasibility of coherent x-ray production by x-ray pumping

We have made calculations which suggest that coherent soft x rays could be produced by inverting the electron population in a target such as Li, through irradiation with x rays generated by fast electrons traversing an electromagnetic field (as in a storage ring). We have derived conditions to be satisfied by target and radiation parameters, and showed that it may be possible to pump LiH adequately with photon pulses that exceed by 2 to 4 orders of magnitude in intensity those now attained in the Stanford Synchrotron Radiation Laboratory, for example.

3.3 Atomic electron binding energies and transition energies from relaxed-orbital relativistic Hartree-Fock-Slater calculations

We have performed complete relativistic relaxed-orbital calculations of neutral-atom binding energies, for all orbitals in all atoms with $2 \leq Z \leq 106$, based on an improved form of the Hartree-Fock-Slater formalism. The Breit interaction (magnetic and retardation) energy is included. A vacuum polarization correction is made; the Uehling potential is listed separately from higher-order contributions. Self-energy shifts for the 1s, 2s, and $2p_{1/2}$ states have also been taken into account. Results agree extremely well with measurements on inner levels of free atoms. Discrepancies with experiment will permit a determination of the influence of many-body effects and of extraatomic relaxation.

The same approach has been used to carry out the first comprehensive computations of the transition energies of all possible L-shell Coster-Kronig processes in all atoms, $11 \leq Z \leq 103$. Cutoffs in Z for various transitions and the effect of quantum-electrodynamic corrections are clearly apparent from

these results. In a first application of these calculations, they permitted us to re-interpret the Ag L x-ray spectrum in a theoretically self-consistent manner.

3.4 X-ray scattering by H_2 and He using synchrotron radiation

Total photon scattering by atoms and molecules is a two-electron expectation value that depends on the average electron-electron separation (by contrast with elastic scattering that depends only upon the radial charge distribution). Most interesting is the application of inelastic photon scattering to study electron correlation in H_2 and He. The cross sections are so small that the experiment cannot be done adequately with conventional x-ray sources. We have performed measurements with synchrotron radiation in the Stanford Synchrotron Radiation Laboratory, covering momentum transfers from 2 to 7 Å^{-1}. The results agree well with theoretical predictions based on correlated wave functions, but disagree substantially with cross sections computed from Hartree-Fock wave functions. Because the scattering measurements distinctly reflect the electron correlation effect, they appear to have promise for a rather direct measure of the correlation energy in various atoms and molecules.

3.5 Reviews of atomic inner-shell processes

A two-volume treatise on atomic inner-shell processes has been edited, providing researchers with a survey of this rapidly developing aspect of atomic physics. A comprehensive review of orbital electron capture by the nucleus, including radiative capture, has been written for the Reviews of Modern Physics.

4. List of Publications

a) Abstracts

1. M. H. Chen and B. Crasemann: Fluorescence Yields of Multiply Ionized Ne and Ar. In Electronic and Atomic Collisions, ed. by J. S. Risley and R. Geballe (U. of Washington Press, Seattle, 1975), Vol. 2, p. 937.

2. D. L. Matthews, R. J. Fortner, M. H. Chen, and B. Crasemann: Sequential Stripping in Highly Ionized Neon. In Electronic and Atomic Collisions, ed. by J. S. Risley and R. Geballe (U. of Washington Press, Seattle, 1975), Vol. 2, p. 941.

3. M. H. Chen, B. Crasemann, L. I Yin, T. Tsang, and I. Adler: Widths of Atomic N-Shell Vacancy States for $46 \leq Z \leq 50$. In Contributed Papers, Second International Conference on Inner-Shell Ionization Phenomena, University of Freiburg, 29 March - 2 April, 1975. (Institute of Physics, University of Freiburg, 1976), p. 208.

4. B. Crasemann: X-Ray Physics after Eighty Years. Keynote Address, in Program and Extended Abstracts, International Conference on the Physics of X-Ray Spectra, August 30 - September 2, 1976. (National Bureau of Standards, Washington, D.C., 1976), p. 1.

5. M. Aoyagi, M. H. Chen, B. Crasemann, K.-N. Huang, and H. Mark: Atomic Electron Binding Energies and Coster-Kronig Energies from Relaxed-Orbital Relativistic Hartree-Fock-Slater Calculations. In R. Marrus, M. H. Prior, and H. A. Shugart, eds., Abstracts, Fifth International Conference on Atomic Physics, Berkeley, California, July 26-30, 1976, p. 300.

6. G. E. Ice and B. Crasemann: Synchrotron-Radiation Measurement of Differential Photon Scattering Cross Sections of H_2. Bull Am. Phys. Soc. 21, 1249 (1976).

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8. B. Crasemann and M. H. Chen: X-Ray and Auger Transition Probabilities to the 2p State of Multiply Ionized Sulfur and Chlorine. In Abstracts of Papers, International Conference on the Physics of Electronic and Atomic Collisions, 10th. (Commissariat a l'Energie Atomique, Paris, 1977), Vol. 1, p. 206.

b) Articles

1. M. H. Chen and B. Crasemann: Multiplet Effects on the $L_{2,3}$ Fluorescence Yield of Multiply Ionized Ar. Phys. Rev. A 10, 2232 (1974).

2. M. H. Chen, B. Crasemann, and D. L. Matthews: K-Shell Fluorescence Yields of Multiply Ionized Ne. Phys. Rev. Lett. 34, 1309 (1975).

3. M. H. Chen and B. Crasemann: Stripping-Mechanism Dependence of the Ar 2s Fluorescence Yield. Phys. Rev. A 12, 710 (1975).

4. P. L. Csonka and B. Crasemann: Feasibility of Coherent X-Ray Production by X-Ray Pumping. Phys. Rev. A 12, 611 (1975).

5. M. H. Chen and B. Crasemann: Auger and Radiative Deexcitation of Multiply Ionized Ne. Phys. Rev. A 12, 959 (1975).

6. M. H. Chen, B. Crasemann, L. I Yin, T. Tsang, and I. Adler: Widths of Atomic 4s and 4p Vacancy States, 46≤Z≤50. Phys. Rev. A 13, 1435 (1976).

7. M. Aoyagi, M. H. Chen, B. Crasemann, K.-N. Huang, and H. Mark: Atomic Electron Energies Including Relativistic Effects and Quantum Electrodynamic Corrections. NASA Technical Report No. NASA TR R-463 (National Technical Information Service, Springfield, Va. 22161).

8. M. Aoyagi, M. H. Chen, B. Crasemann, K.-N. Huang, and H. Mark: Relativistic Electrostatic Slater Integrals, 2≤Z≤106. NASA Technical Report No. NASA TR R-464 (National Technical Information Service, Springfield, Va. 22161).

9. K.-N. Huang, M. Aoyagi, M. H. Chen, B. Crasemann, and H. Mark: Neutral-Atom Electron Binding Energies from Relaxed-Orbital Relativistic Hartree-Fock-Slater Calculations, 2≤Z≤106. Atomic Data and Nuclear Data Tables 18, 243 (1976).

10. K.-N. Huang: Correlated Wave Functions for Three-Particle Systems with Coulomb Interaction - The Muonic Helium Atom. Phys. Rev. A 15, 1832 (1977).

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13. M. H. Chen, B. Crasemann, K.-N. Huang, M. Aoyagi, and H. Mark: Theoretical L-Shell Coster-Kronig Energies $11 \leq Z \leq 103$. Atomic Data and Nuclear Data Tables 19, 97 (1977).

14. M. H. Chen: Auger and Radiative Deexcitation of the $1s2\ell3\ell'$ Configurations of Lithium-Like Neon. Phys. Rev. A 15, 2318 (1977).

15. D. Ton-That: Target-ℓ Convergence Rates of Certain Atomic (Radial) Matrix Elements with Application to ℓ' Dependence of $n\ell n'\ell'$ Excitation in Direct Scattering. Submitted to Phys. Rev. A.

16. D. Ton-That and M. R. Flannery: On Populating ℓ' States in Intermediate-Impact-Energy, Direct-Scattering $n\ell n'\ell'$ Excitation. Submitted to Phys. Rev. A.

17. M. H. Chen and B. Crasemann: X-Ray and Auger Transition Probabilities to the 2p Level of Multiply Ionized Sulfur and Chlorine. Phys. Rev. A, in press.

18. G. E. Ice, M. H. Chen, and B. Crasemann: Photon Scattering Cross Sections of H_2 and He Measured with Synchrotron Radiation. Phys. Rev. A, in press.

c) Book

1. B. Crasemann, ed.: Atomic Inner-Shell Processes. Academic Press, New York, 1975. 2 vols.

5. Scientific Personnel

Bernd Crasemann, Professor of Physics, Principal Investigator.

Mau Hsiung Chen, Adjunct Assistant Professor of Physics, Research Associate.

Gene E. Ice, Research Associate (from June 1, 1977). (Research Assistant to May 31, 1977. Ph.D. awarded June, 1977).

Keh-Ning Huang, Research Associate (October 15, 1974 to November 30, 1976).

Dinh Ton-That, Research Associate (November 1, 1976 to October 1, 1977).

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Osuk Kwon, Research Assistant (Summer, 1975).

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